APPROVED O.G. FIG.
BY CLASS SUBCLASS
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Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov *et al.*; Tel: 202/371-2600
Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries

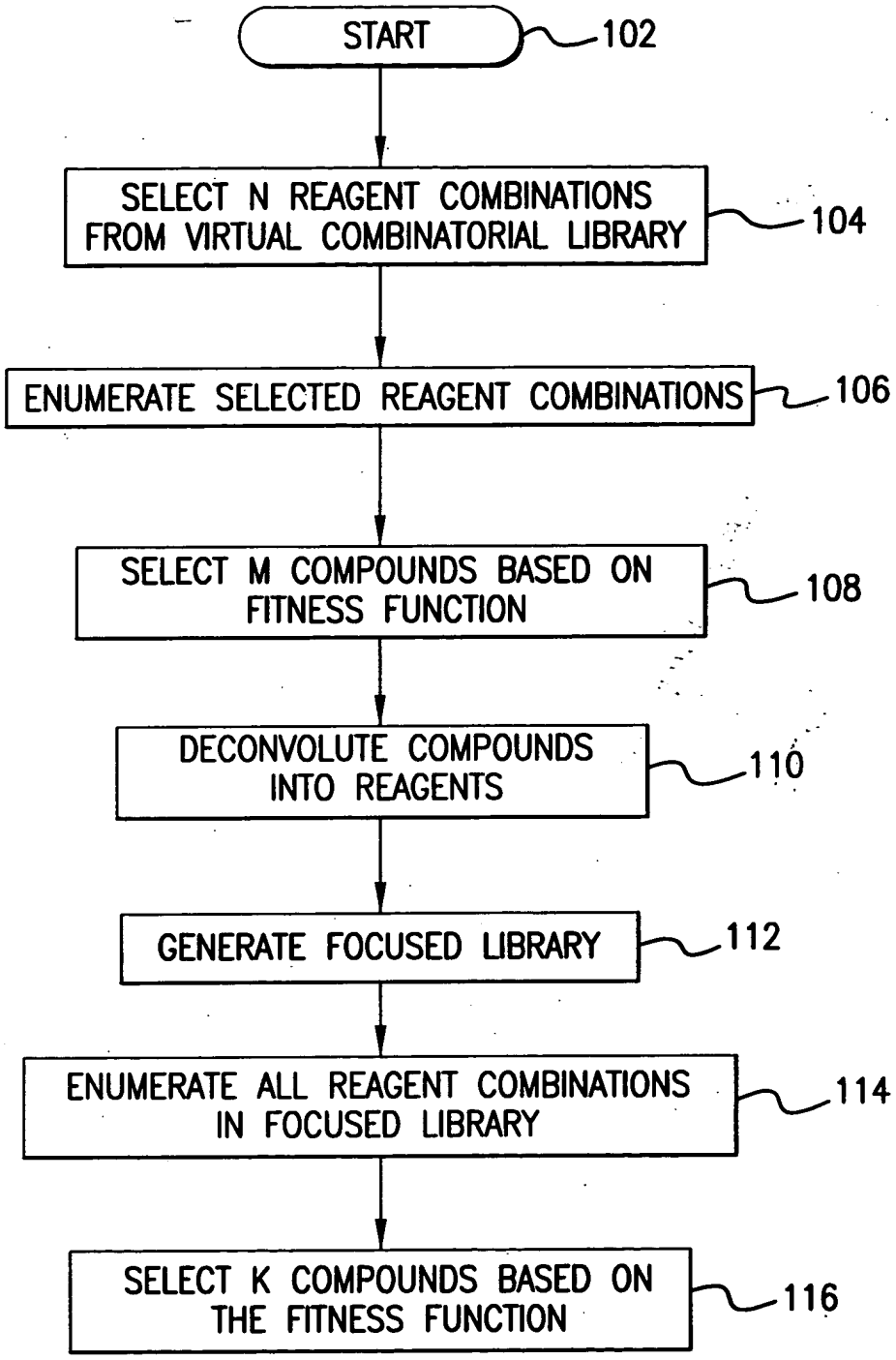

FIG.1

APPROVED O.G. FIG.
BY CLASS SUBCLASS
DRAFTSMAN

Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov *et al.*; Tel: 202/371-2600
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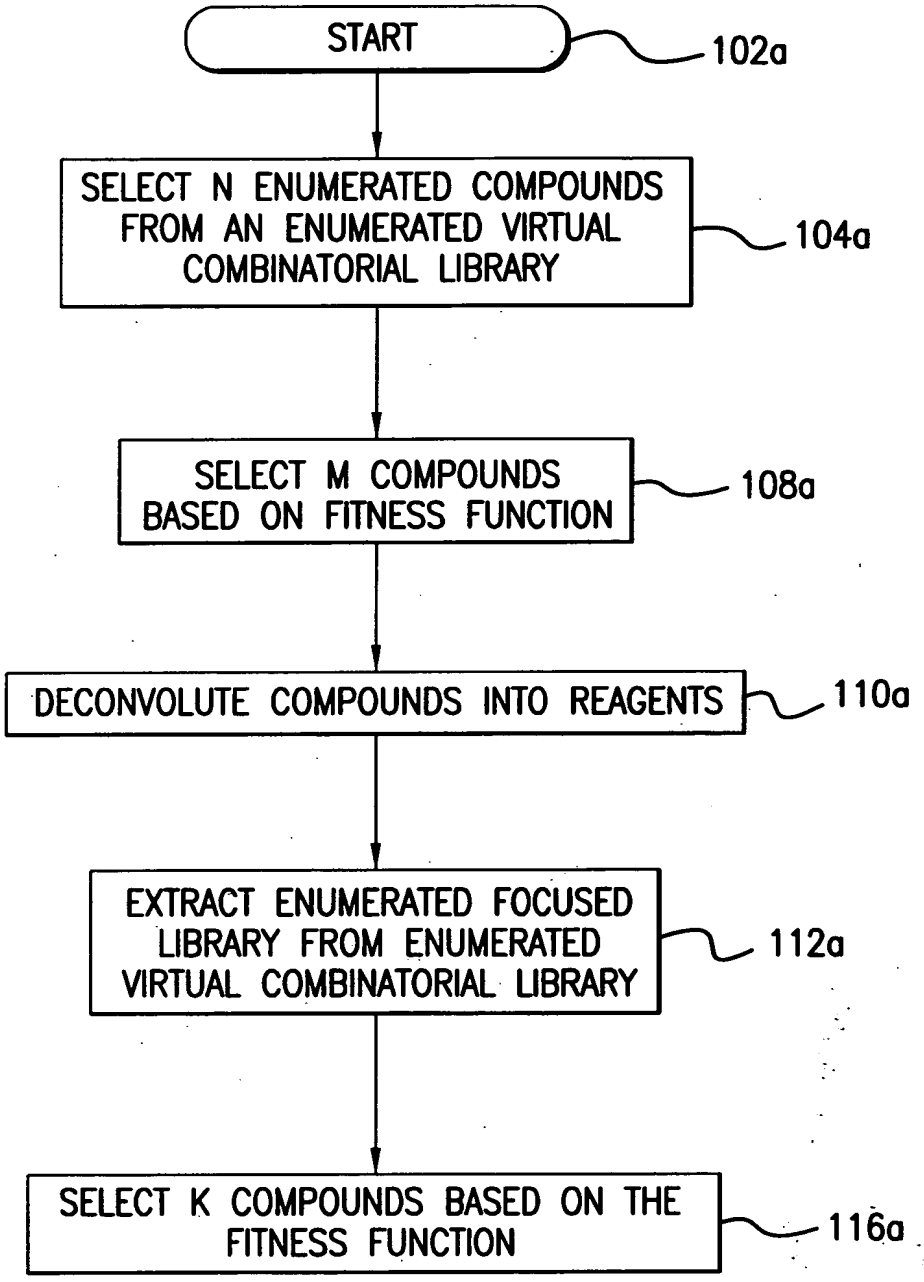

FIG.1A

APPROVED O.G. FIG.
BY
DRAFTSMAN
CLASS SUBCLASS

Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov *et al.*; Tel: 202/371-2600
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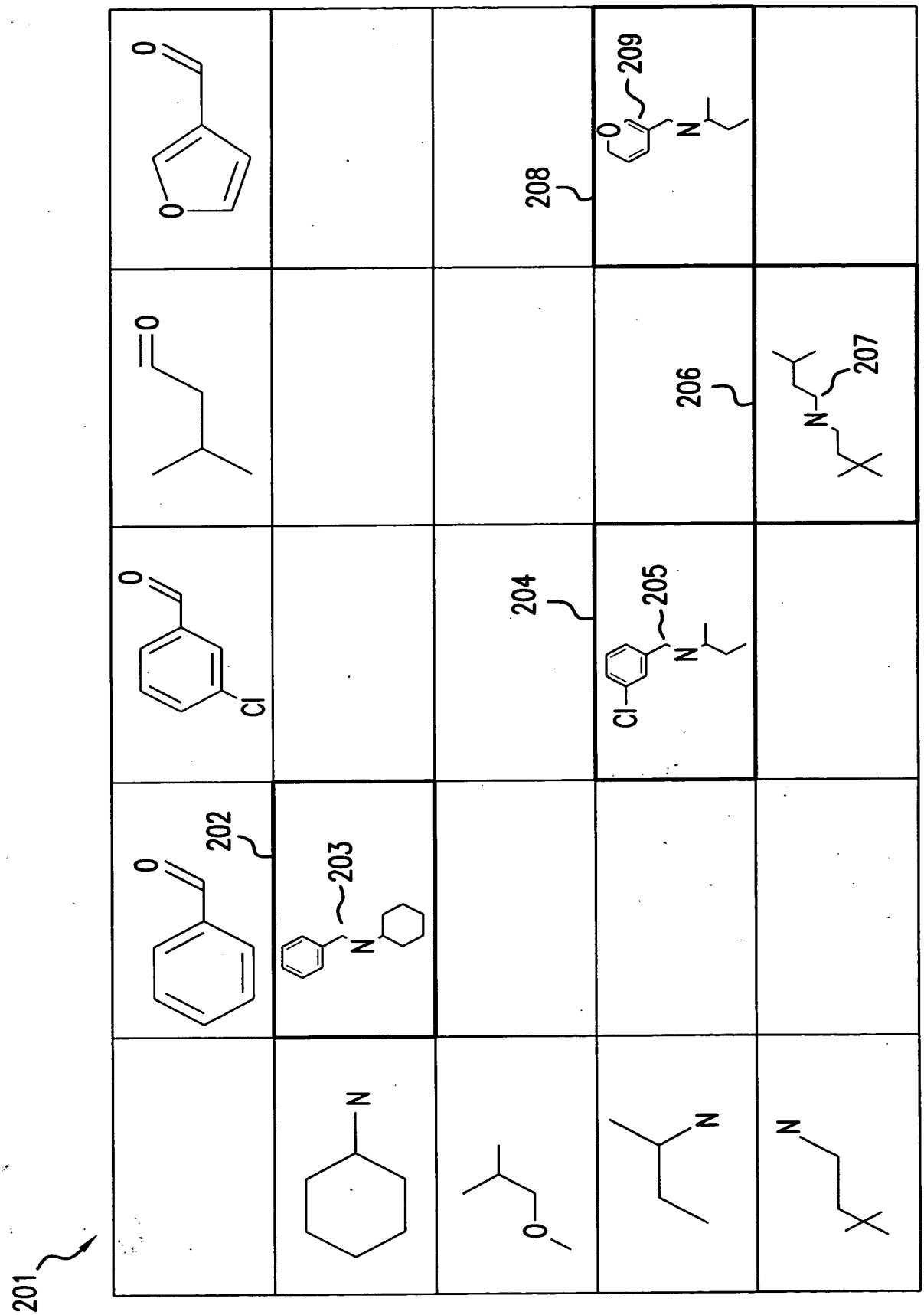

FIG.2

APPROVED O.G. FIG.
BY CLASS SUBCLASS
DRAFTSMAN

Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov *et al.*; Tel: 202/371-2600
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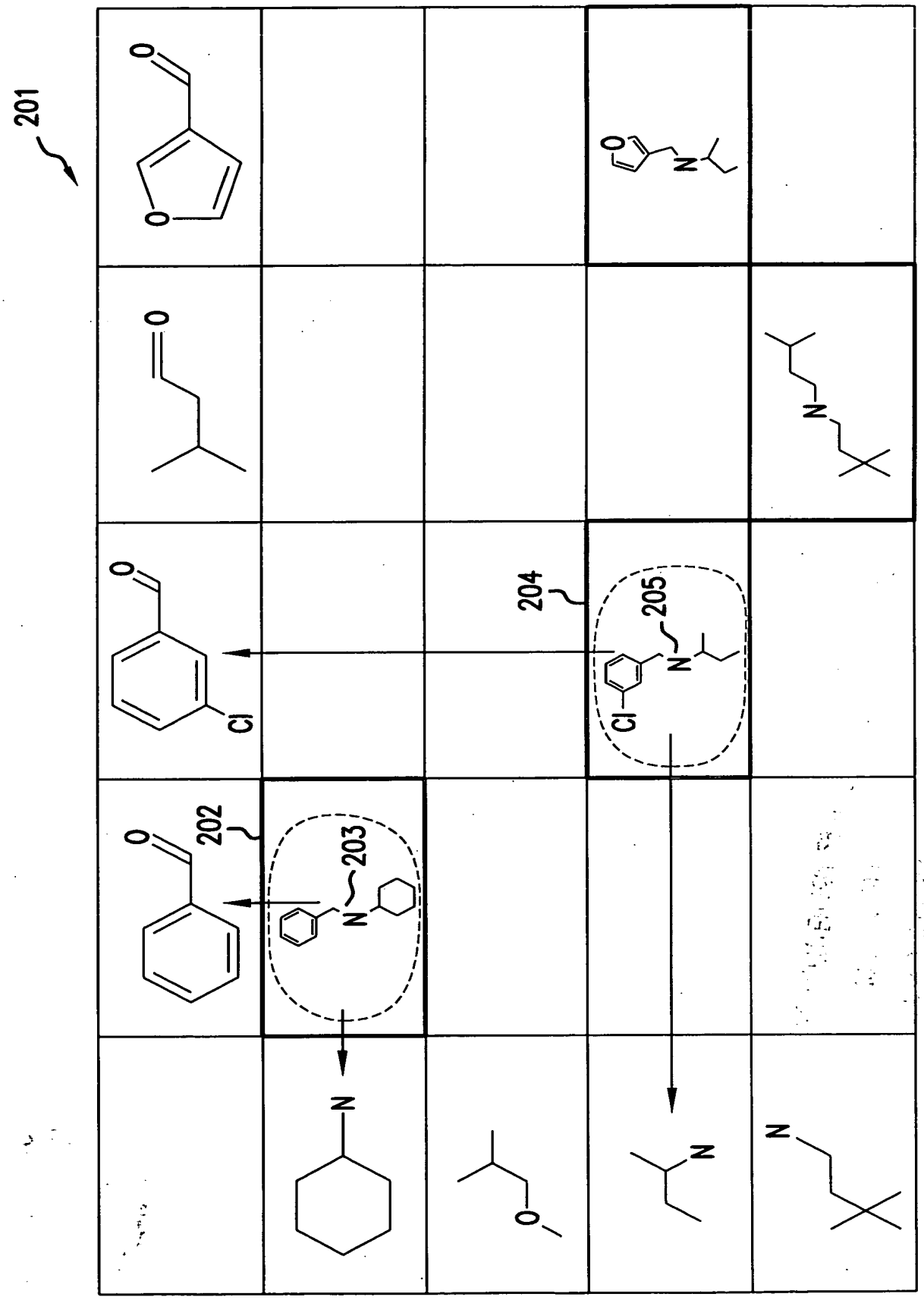
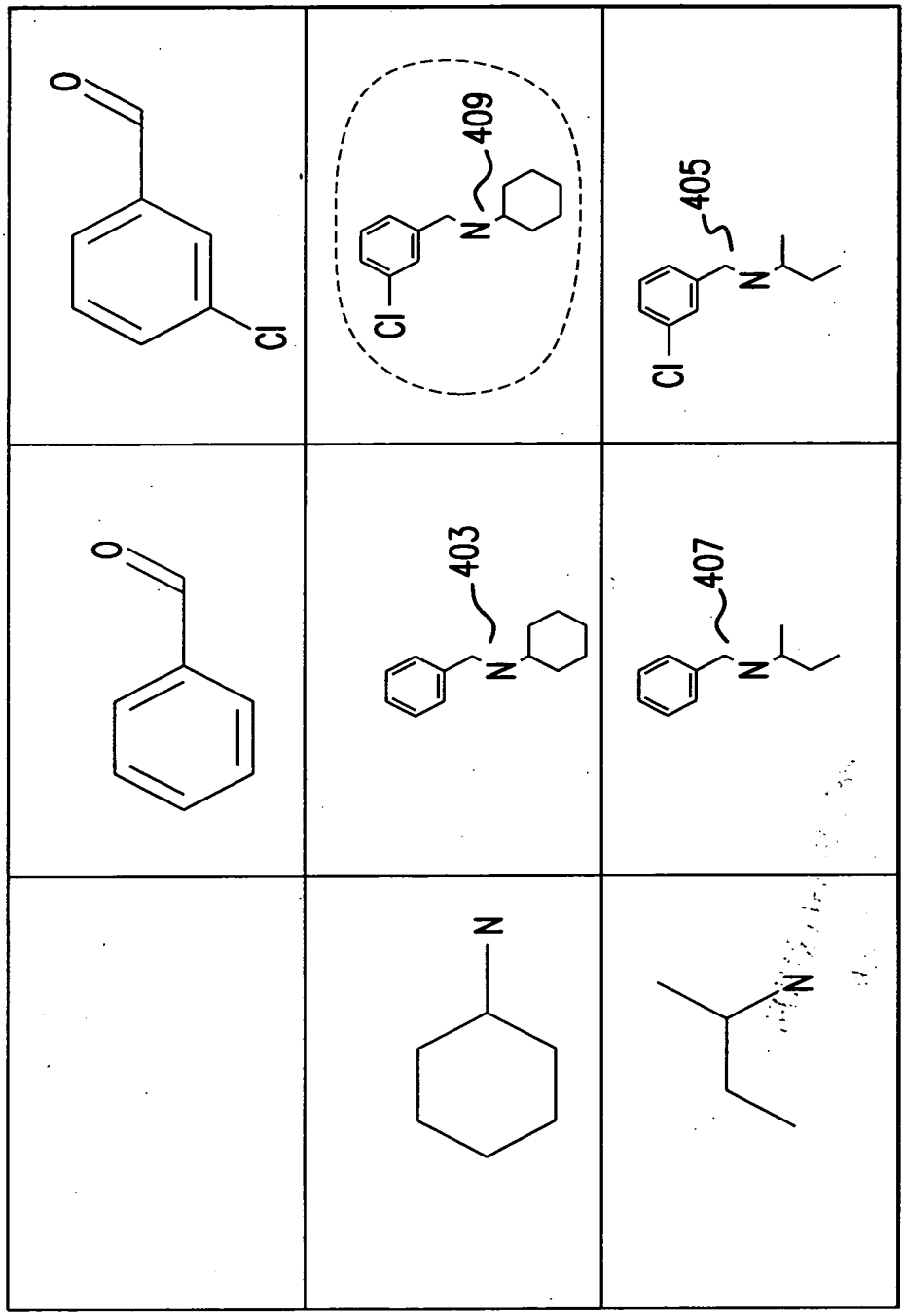


FIG.3

APPROVED O G. FIG.
BY CLASS SUBCLASS
DRAFTSMAN

Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov *et al.*; Tel: 202/371-2600
Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries



401

FIG.4

APPROVED O.G. FIG.
BY CLASS SUBCLASS
DRAFTSMAN

Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov *et al.*; Tel: 202/371-2600
Title: System, Method and Computer Program Product for [illegible] and Efficient Searching of Large Chemical Libraries

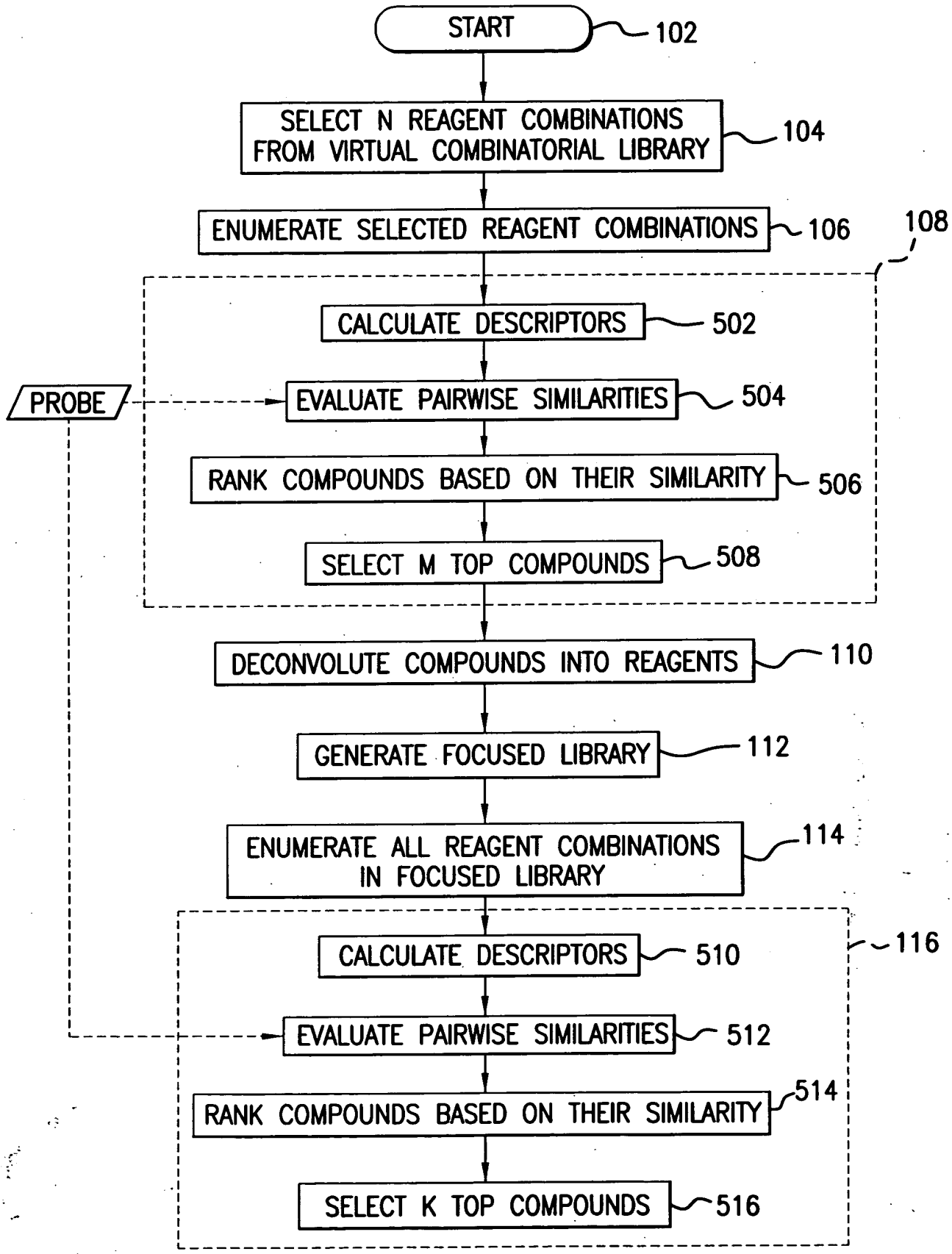


FIG.5

APPROVED O.G. FIG.
BY CLASS SUBCLASS
DRAFTSMAN

Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov *et al.*; Tel: 202/371-2600
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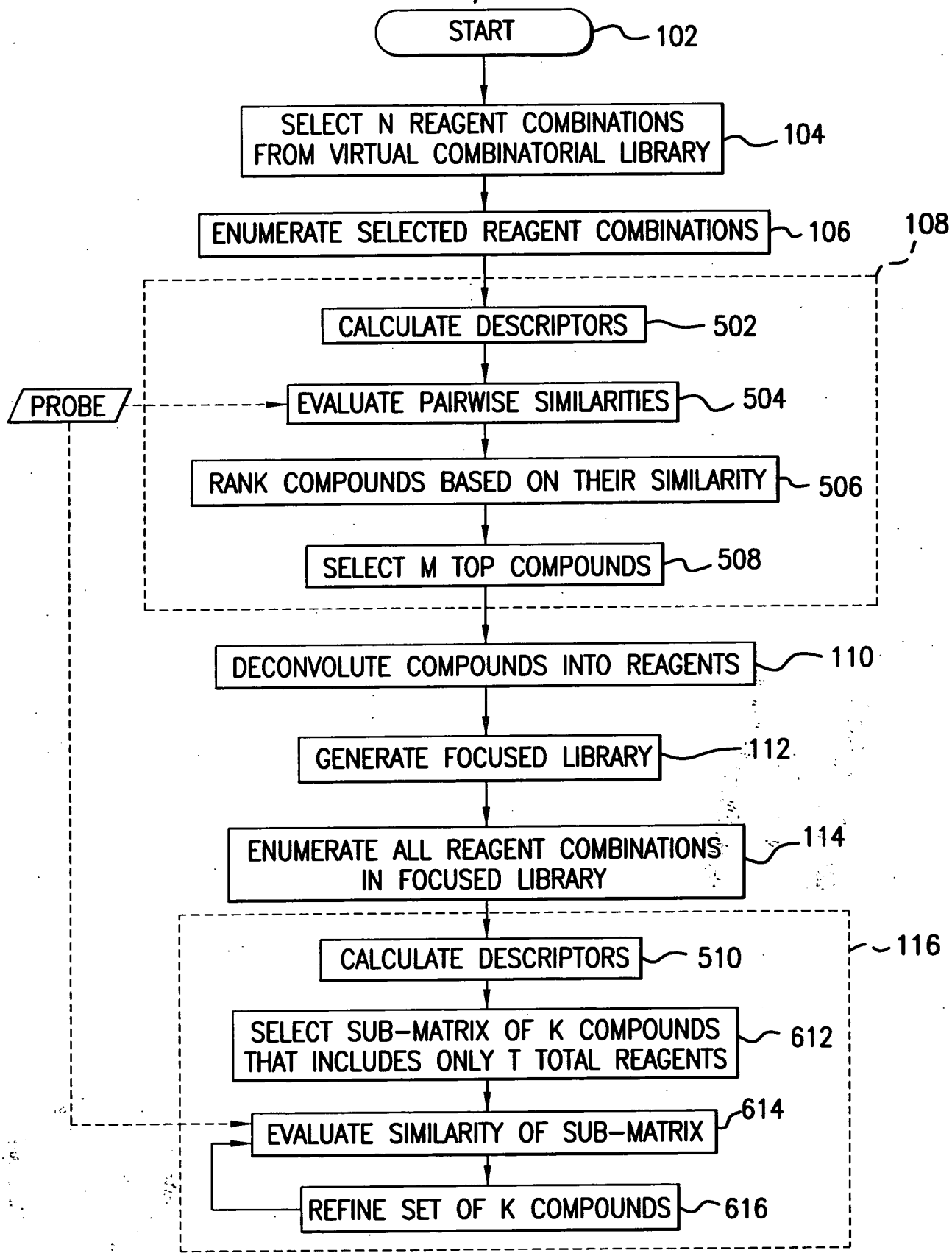

FIG.6

APPROVED O.G. FIG.
BY CLASS SUBCLASS
DRAFTSMAN

Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov *et al.*; Tel: 202/371-2600
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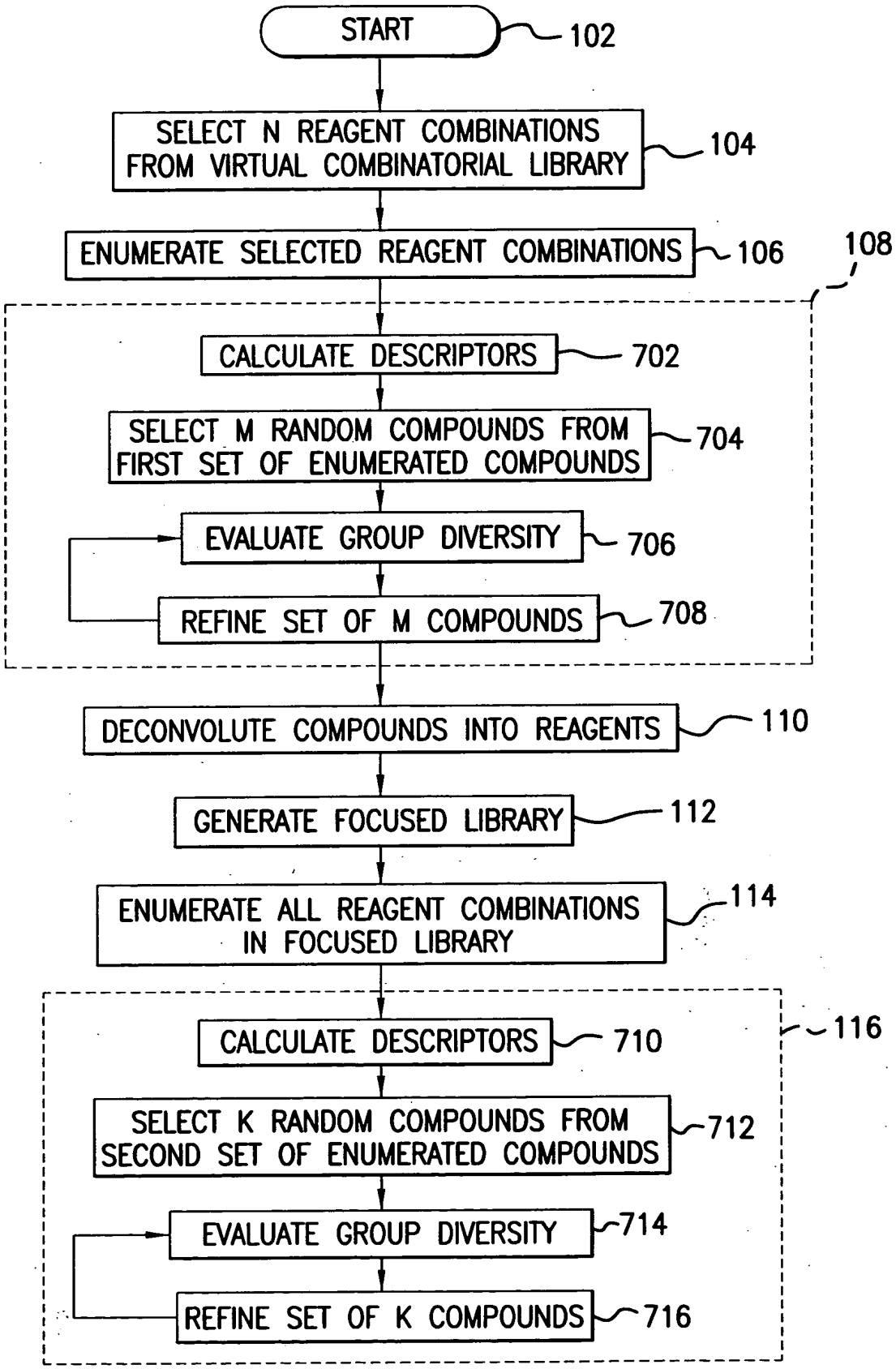

FIG.7

APPROVED O.G. FIG.
BY CLASS SUBCLASS
DRAFTSMAN

Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov *et al.*; Tel: 202/371-2600
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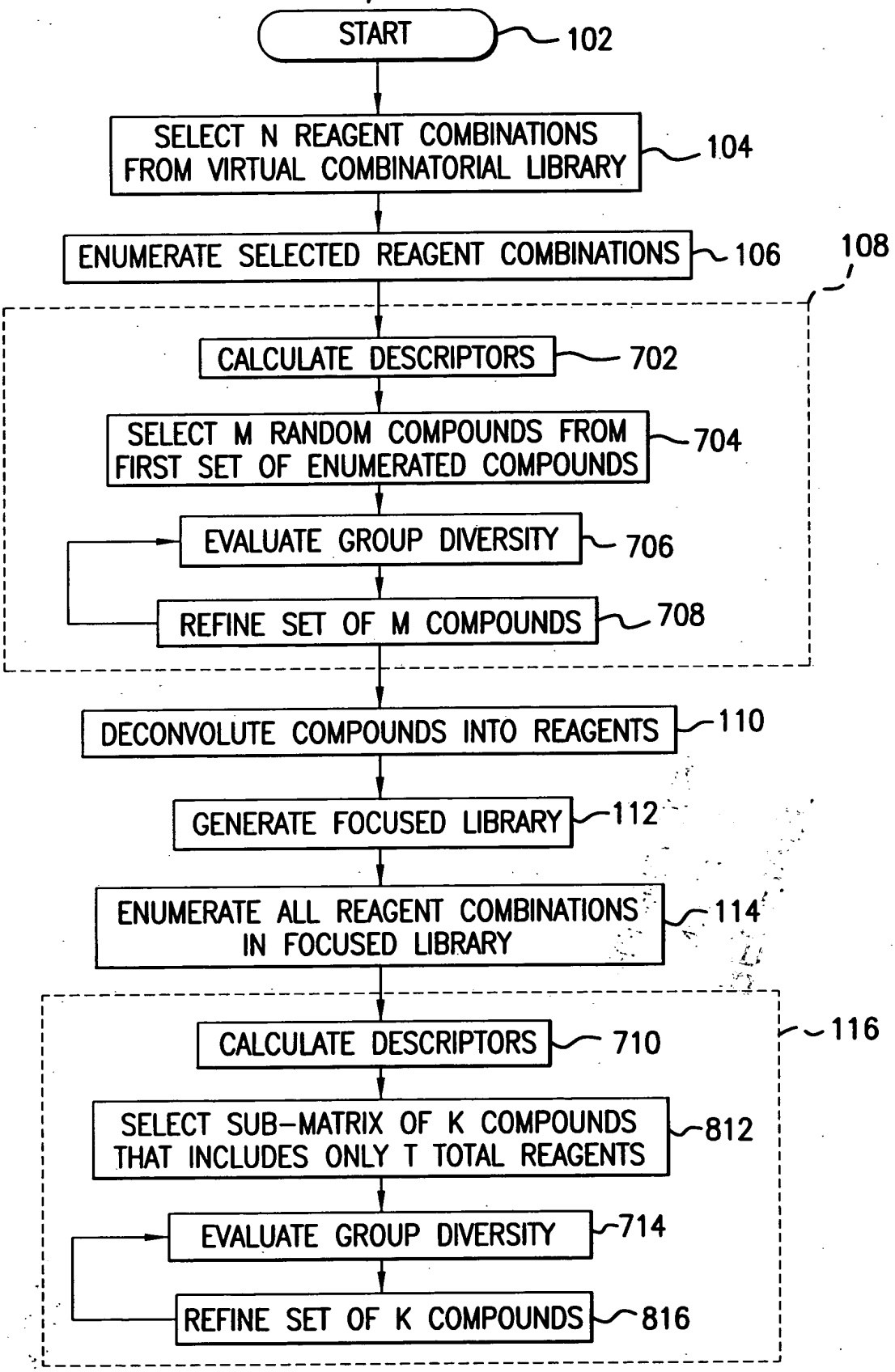

FIG.8

APPROVED O G. FIG.
BY CLASS SUBCLASS
DRAFTSMAN

Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov *et al.*; Tel: 202/371-2600
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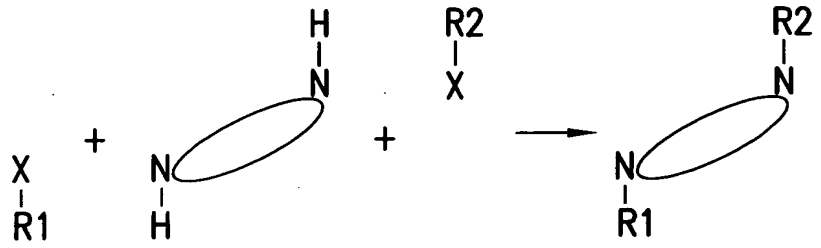


FIG.9A

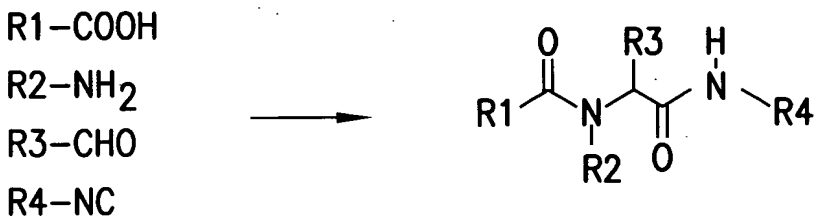
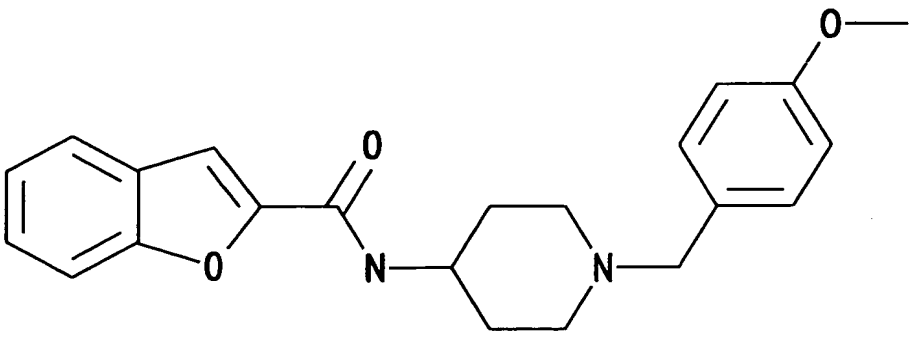


FIG.9B

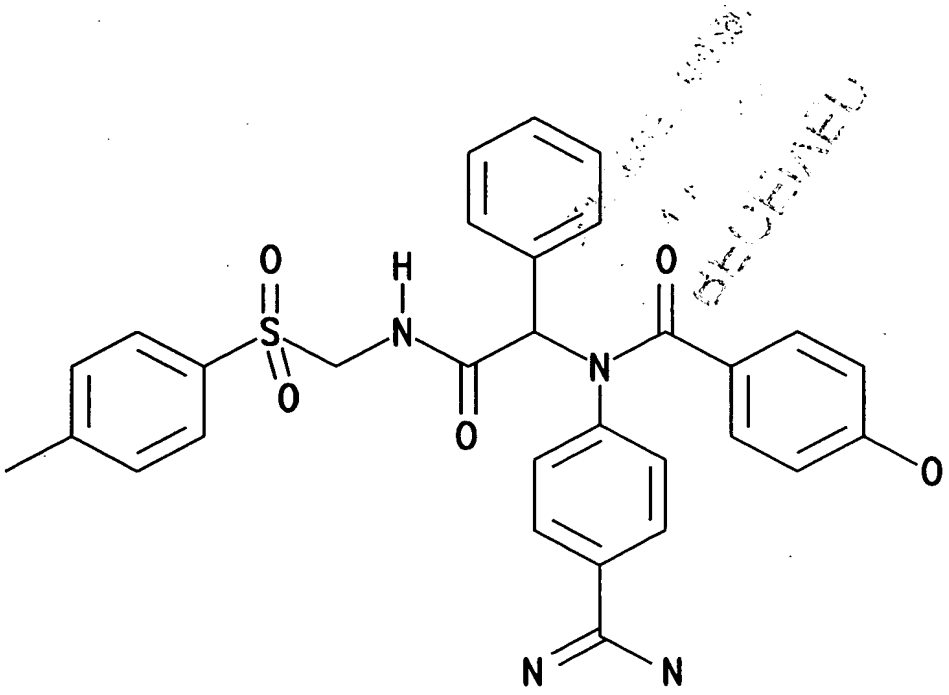
APPROVED O.G. FIG.
BY CLASS SUBCLASS
DRAFTSMAN

Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov *et al.*; Tel: 202/371-2600
Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries



ANTIARRHYTHMIC AGENT

FIG.10A



1.4 M THROMBIN INHIBITOR

FIG.10B

APPROVED O.G. FIG.
BY CLASS SUBCLASS
DRAFTSMAN

Appl. No. 09/506,741; Group Art Unit: 1631
[illegible]t. No. 1503.0730000;
[illegible]ventor(s): Lobanov *et al.*; Tel: 202/371-2600
Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries

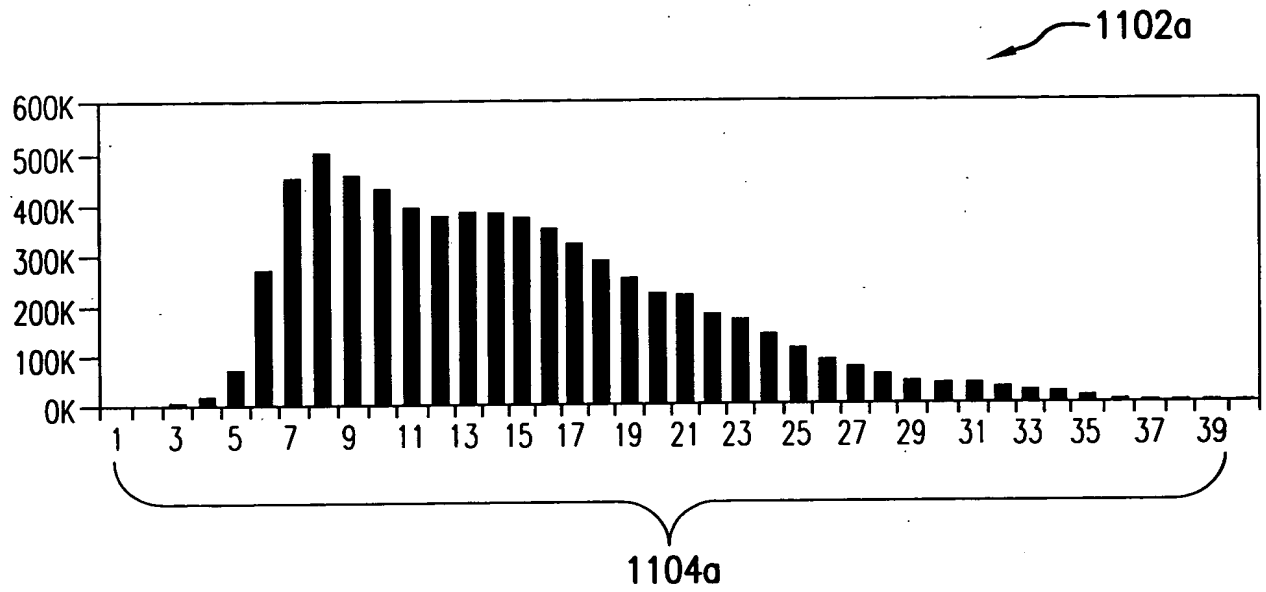


FIG.11A

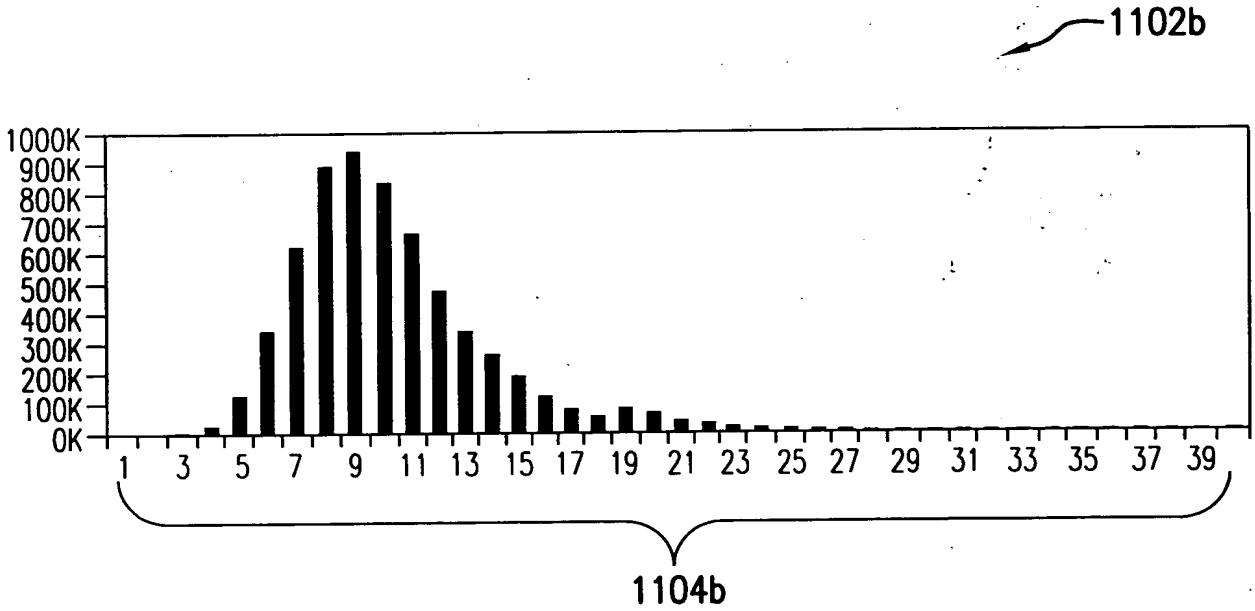


FIG.11B

APPROVED O.G. FIG.
BY CLASS SUBCLASS
DRAFTSMAN

Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov *et al.*; Tel: 202/371-2600
Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries

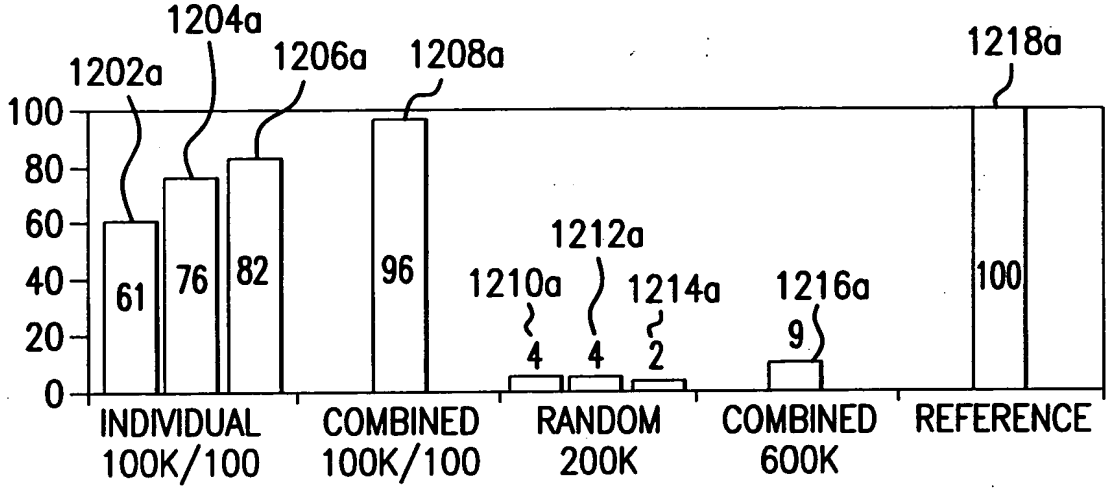


FIG.12A

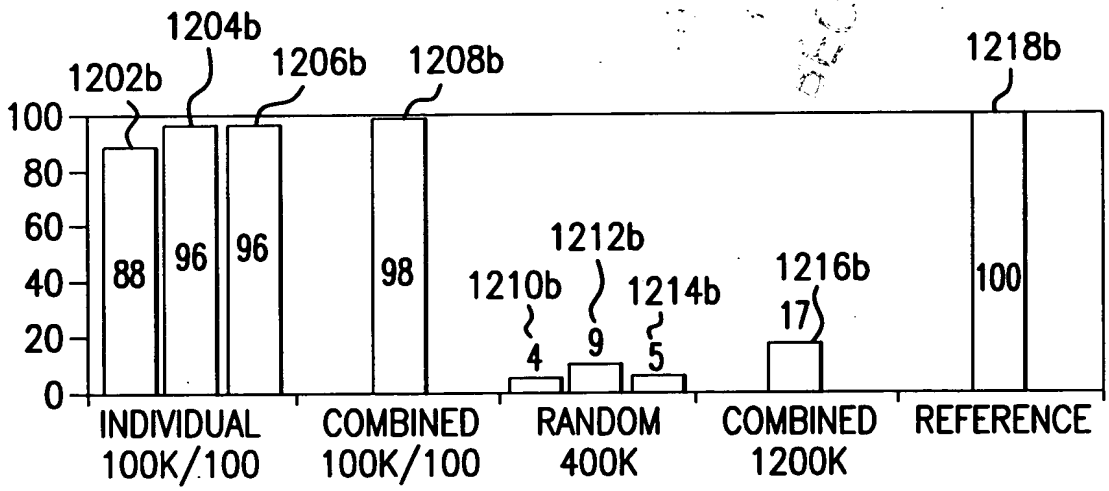


FIG.12B

APPROVED O.G. FIG.
BY CLASS SUBCLASS
DRAFTSMAN

Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov *et al.*; Tel: 202/371-2600
Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries

FIG. 13

1302

	SIZE OF RANDOM SELECTION	NUMBER OF TOP RANKED COMPOUNDS SELECTED	BEST SIMILARITY SCORE	NUMBER OF REAGENTS	SIZE OF FOCUSED LIBRARY	NUMBER OF MOST SIMILAR COMPOUNDS SELECTED	BEST SIMILARITY SCORE	AVERAGE SIMILARITY SCORE	PERCENT OF TOP 100 FOUND	TOTAL COMPOUNDS SCREENED	PERCENT OF THE LIBRARY SCREENED
DIAMINE LIBRARY	N/A	100	0.7662	38	N/A	100	0.7662	1.30034	100	6750000	100
100K/10	100000	10	1.0207	20	300	100	0.8585	1.48825	37	300900	4
100K/50	100000	50	1.2266	70	12896	100	0.7662	1.31148	88	338688	5
100K/100	100000	100	1.0207	108	47487	100	0.7662	1.30306	96	442461	7
100K/200	100000	200	0.7662	167	170959	100	0.7662	1.30034	100	812877	12
1K/100	1000	100	2.1172	195	276623	100	0.7662	1.32782	88	832869	12
10K/100	**10000**	**100**	**1.6919**	**151**	**126249**	**100**	**0.7662**	**1.30141**	**98**	**408747**	**6**
100K/100	100000	100	1.0207	108	47487	100	0.7662	1.30306	96	442461	7
200K/100	200000	100	1.4557	96	33032	100	0.7662	1.30306	96	699096	10
RANDOM 200K	200000	100	1.1272	N/A	N/A	100	1.1272	1.82826	9	600000	9
Ugi LIBRARY	N/A	100	0.0000	37	N/A	100	0.0000	1.47494	100	6290000	100
100K/10	100000	10	0.7745	23	1153	100	0.7745	1.78473	46	303459	5
100K/50	**100000**	**50**	**1.6871**	**76**	**96234**	**100**	**0.0000**	**1.47494**	**100**	**588702**	**9**
100K/100	100000	100	1.4382	99	267251	100	0.0000	1.47737	98	1101753	18
100K/200	100000	200	1.1581	139	843712	100	0.0000	1.47737	98	2831136	45
1K/100	1000	100	2.5500	151	1300555	100	0.0000	1.47494	100	3904665	62
10K/100	10000	100	1.3793	121	583482	100	0.0000	1.48308	97	1780446	28
100K/100	100000	100	1.4382	99	267251	100	0.0000	1.47737	98	1101753	18
200K/100	200000	100	0.77448	96	222673	100	0.0000	1.47494	100	1268019	20
1K/50	1000	50	2.50076	102	331653	100	0.0000	1.52529	86	997959	16
10K/50	10000	50	1.22499	88	190661	100	0.0000	1.49912	92	601983	10
100K/50	100000	50	1.6871	76	96234	100	0.0000	1.47494	100	588702	9
200K/50	200000	50	1.1667	68	68089	100	0.0000	1.48086	98	804267	13
RANDOM 400K	400000	100	0.0000	N/A	N/A	100	0.0000	2.18251	17	1200000	19

1304 1306 1308 1310

APPROVED O.G. FIG.
BY CLASS SUBCLASS
DRAFTSMAN

Appl. No. 09/506,741; Group Art Unit: 1631
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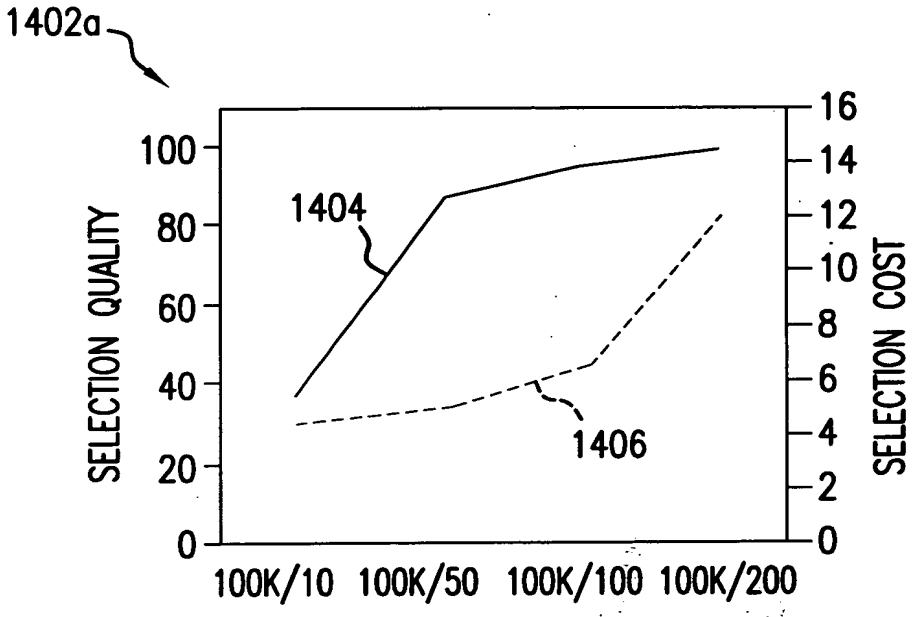

FIG.14A

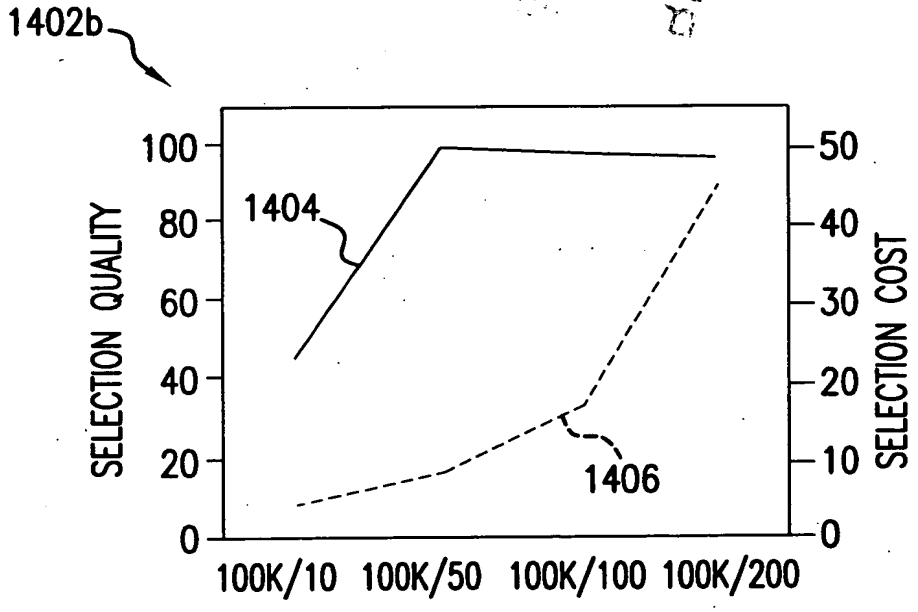

FIG.14B

APPROVED O.G. FIG.
BY CLASS SUBCLASS
DRAFTSMAN

Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
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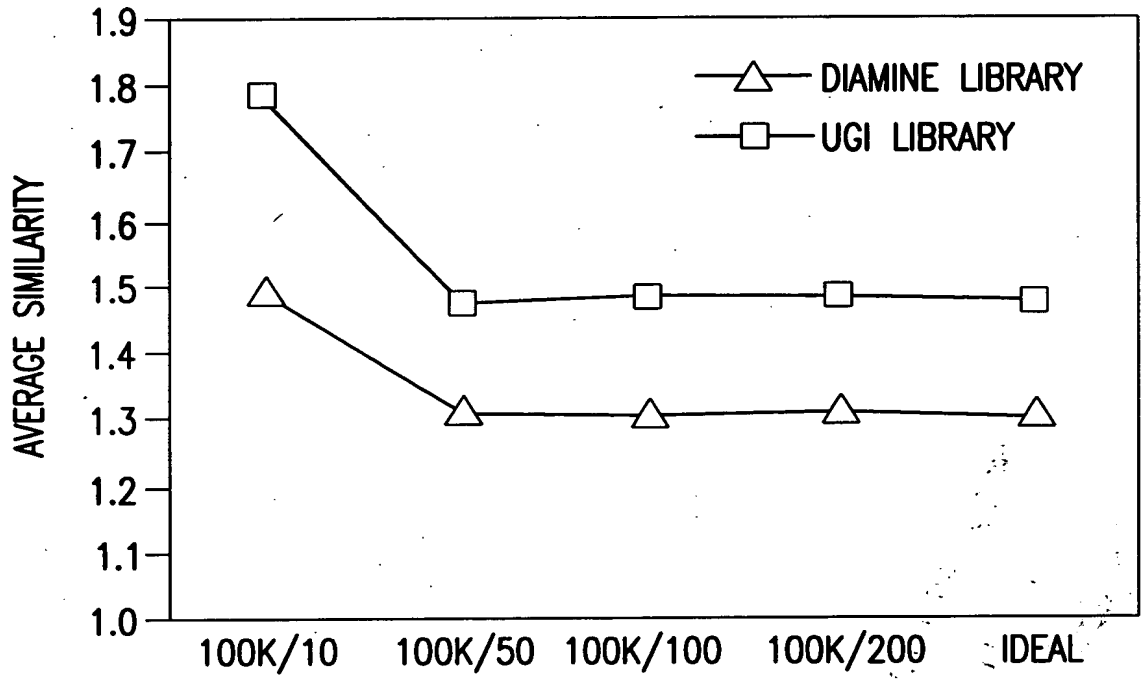

FIG.15

APPROVED | O.G. FIG.
BY | CLASS | SUBCLASS
DRAFTSMAN

Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov *et al.*; Tel: 202/371-2600
Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries

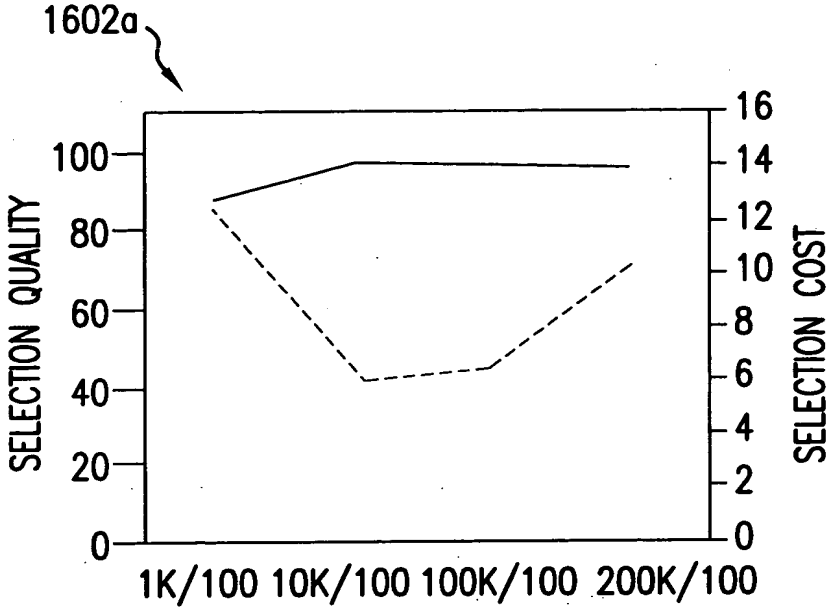

FIG.16A

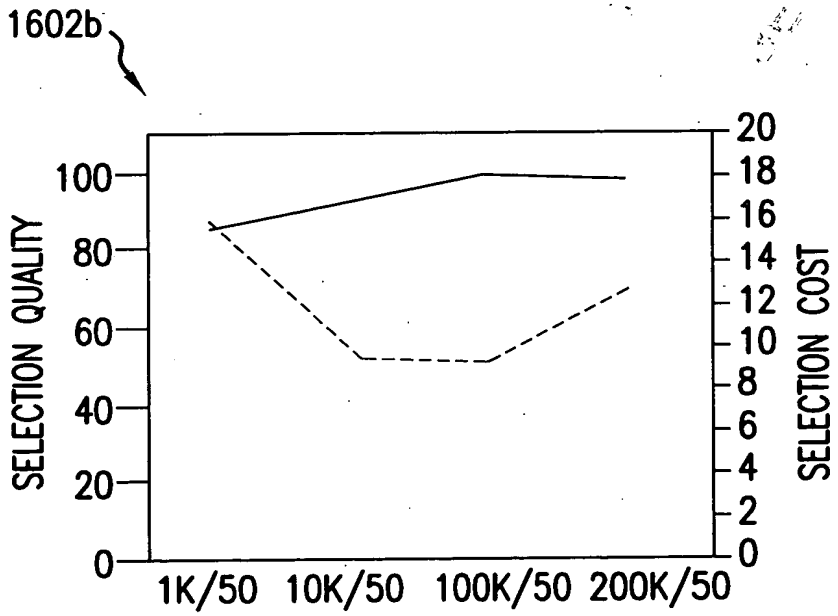

FIG.16B

APPROVED | O.G. FIG.
BY | CLASS | SUBCLASS
DRAFTSMAN

Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov *et al.*; Tel: 202/371-2600
Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries

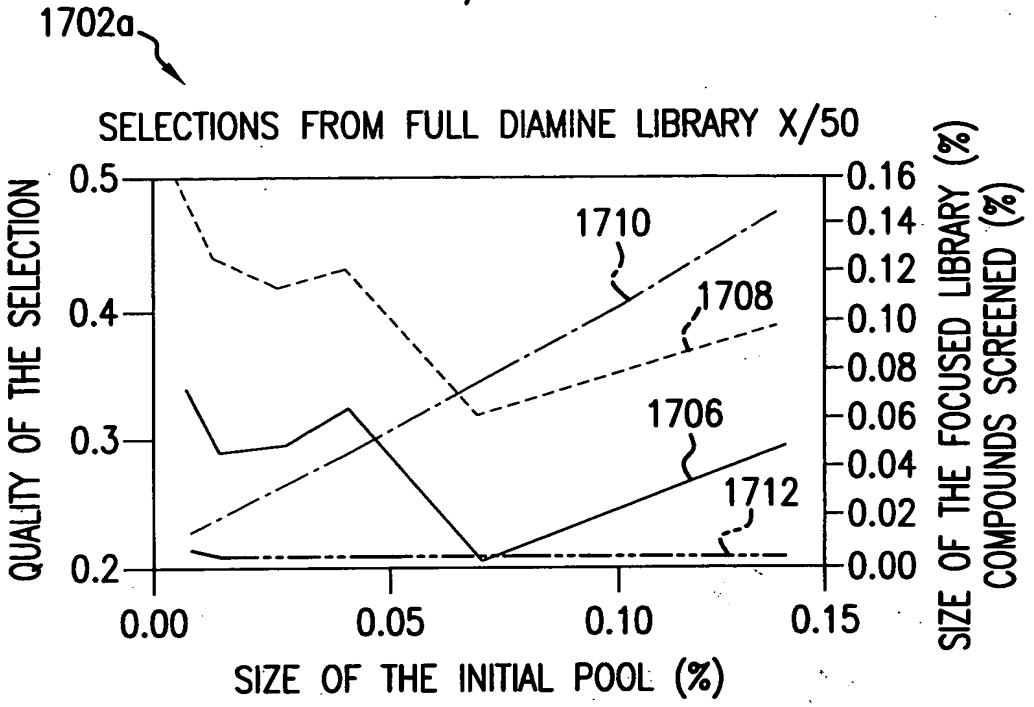

FIG.17A

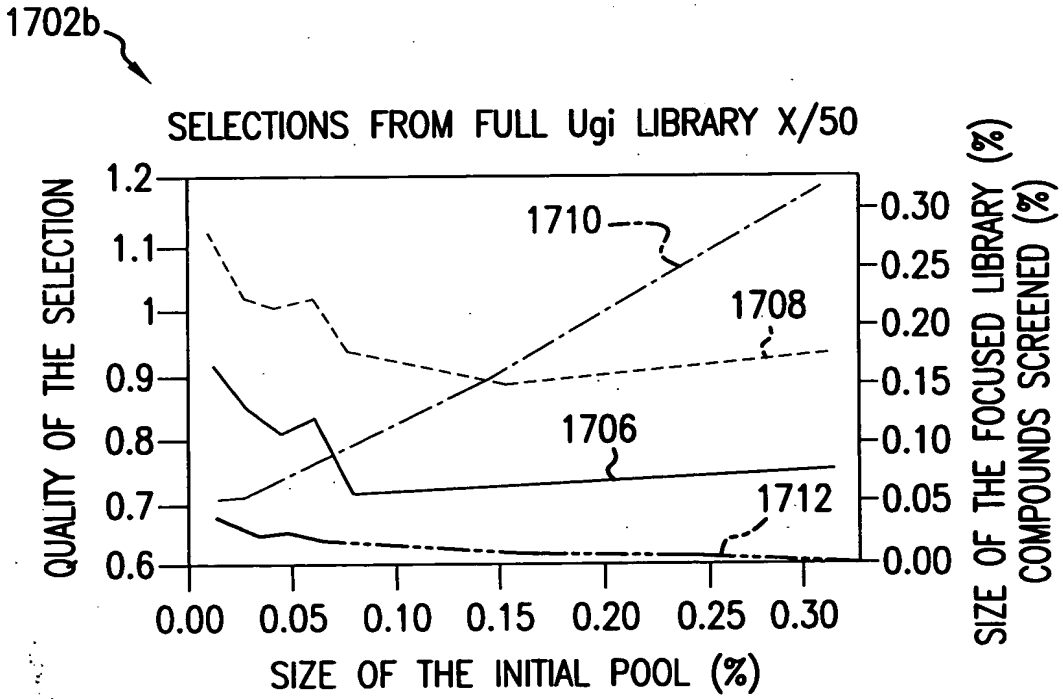

FIG.17B

APPROVED | O.G. FIG.
BY | CLASS | SUBCLASS
DRAFTSMAN

Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov *et al.*; Tel: 202/371-2600
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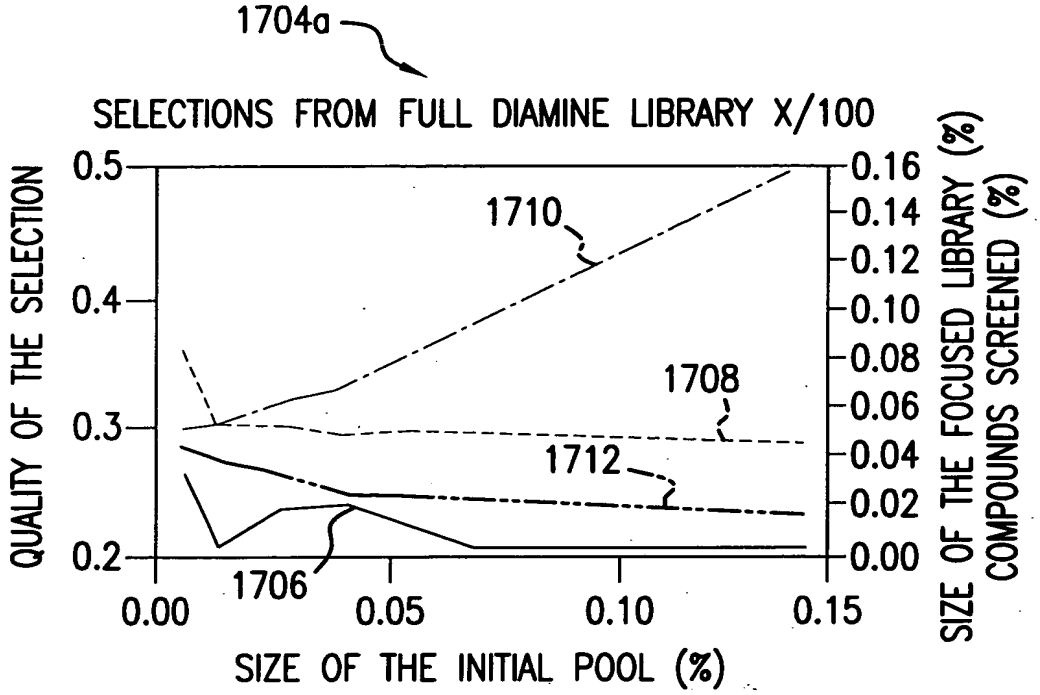


FIG.17C

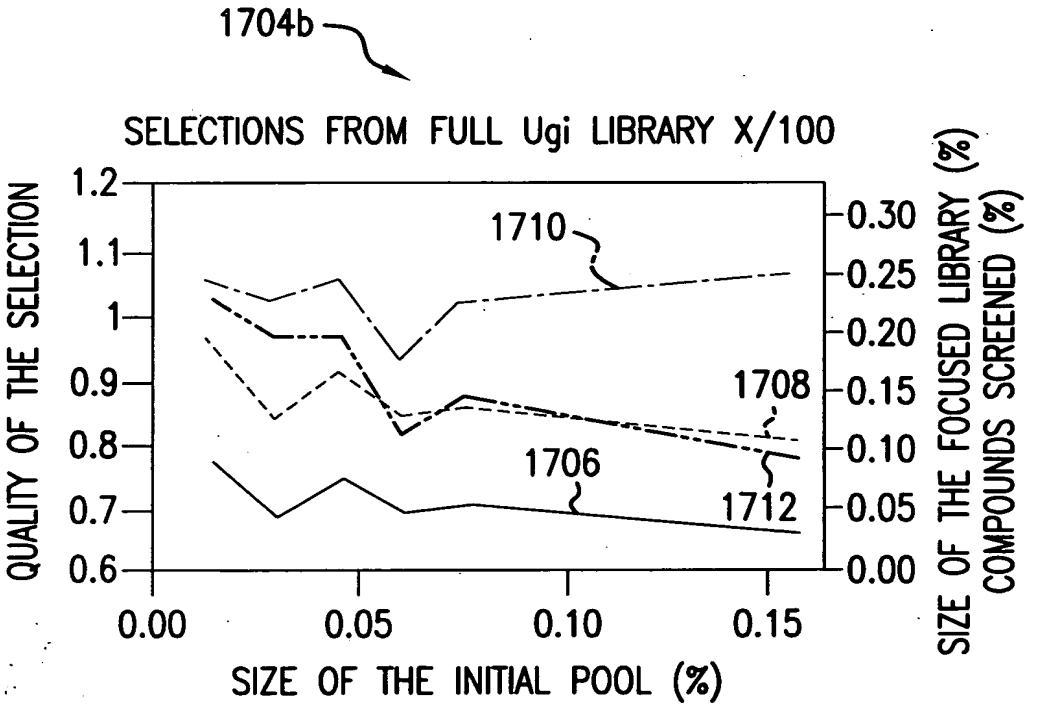
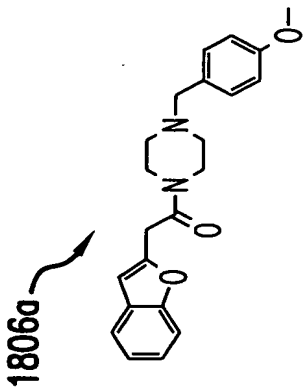
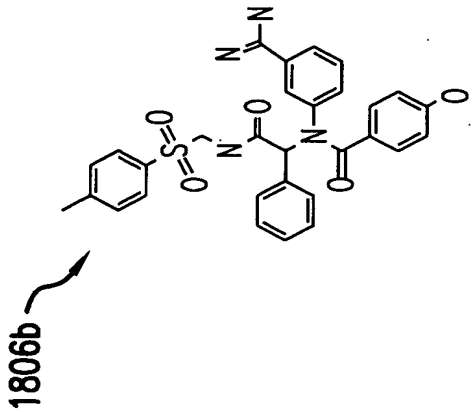


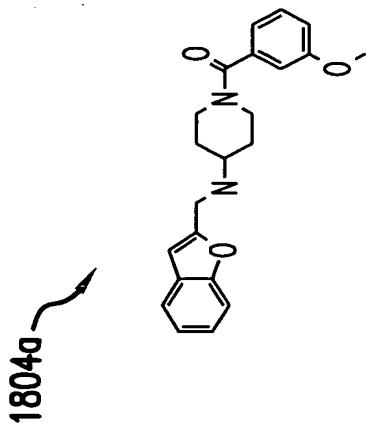
FIG.17D

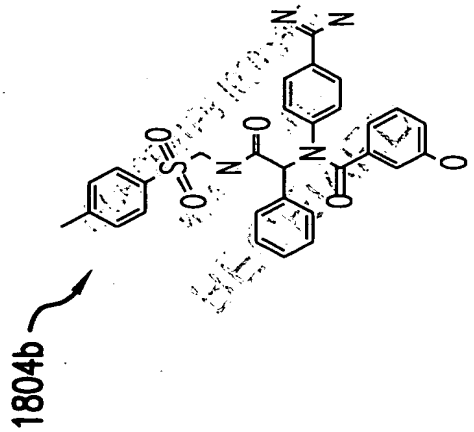
APPROVED O.G. FIG.
BY CLASS SUBCLASS
DRAFTSMAN

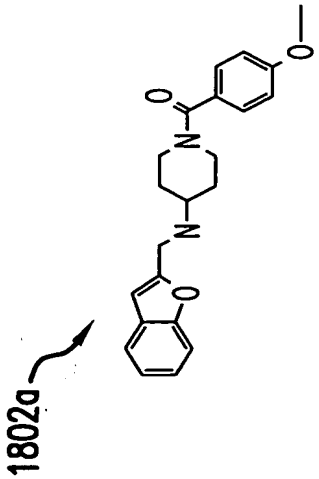
Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov *et al.*; Tel: 202/371-2600
Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries











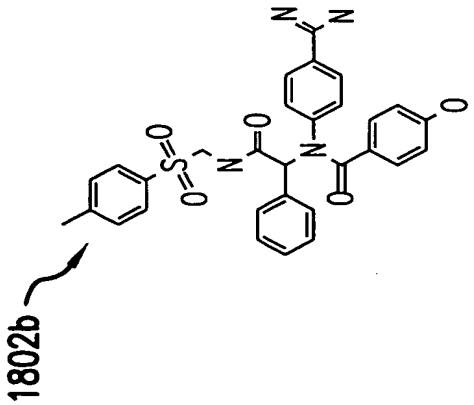


FIG.18

APPROVED O.G. FIG.
BY CLASS SUBCLASS
DRAFTSMAN

Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov *et al.*; Tel: 202/371-2600
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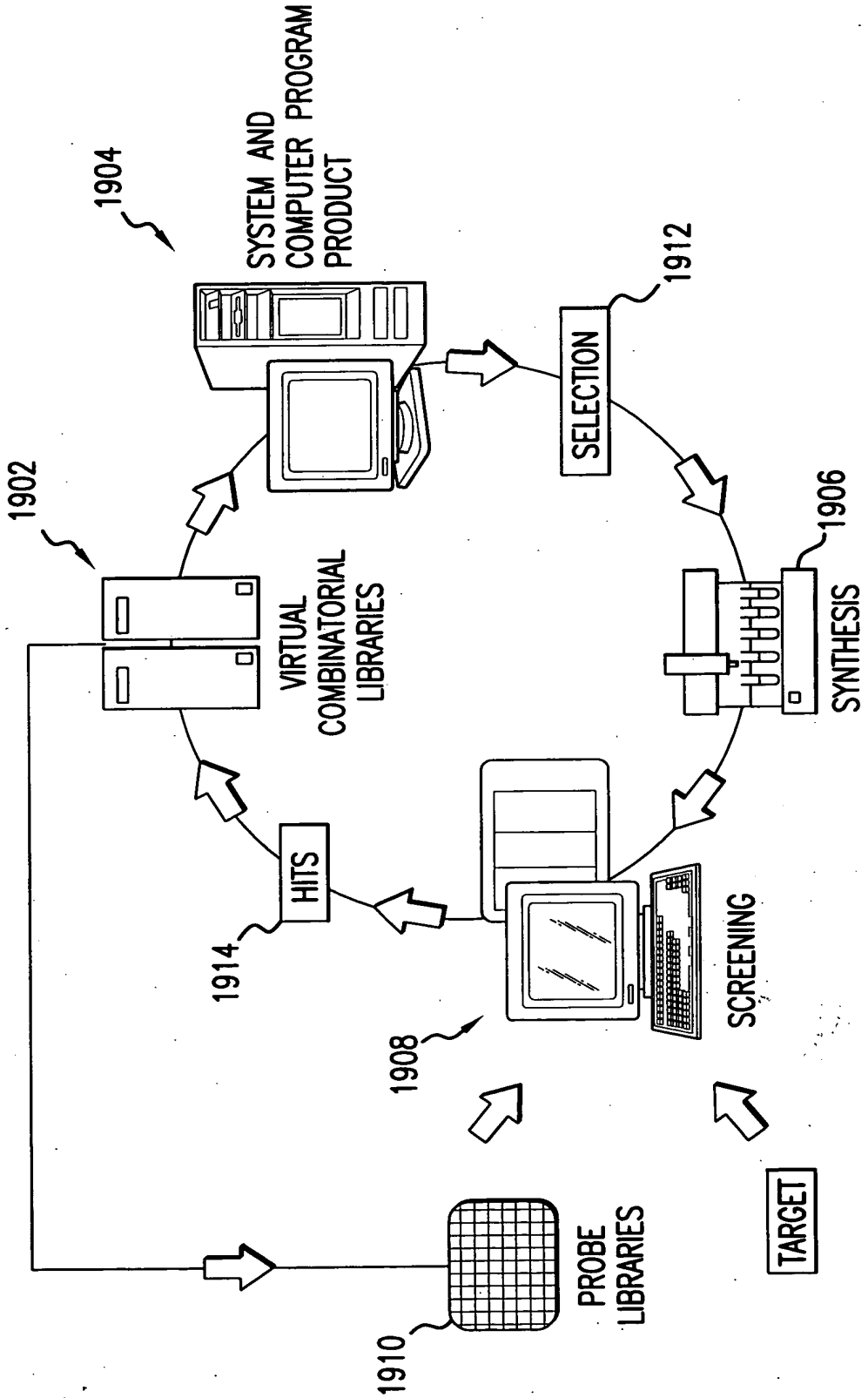

FIG.19

APPROVED O.G. FIG.
BY CLASS SUBCLASS
DRAFTSMAN

Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov *et al.*; Tel: 202/371-2600
Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries

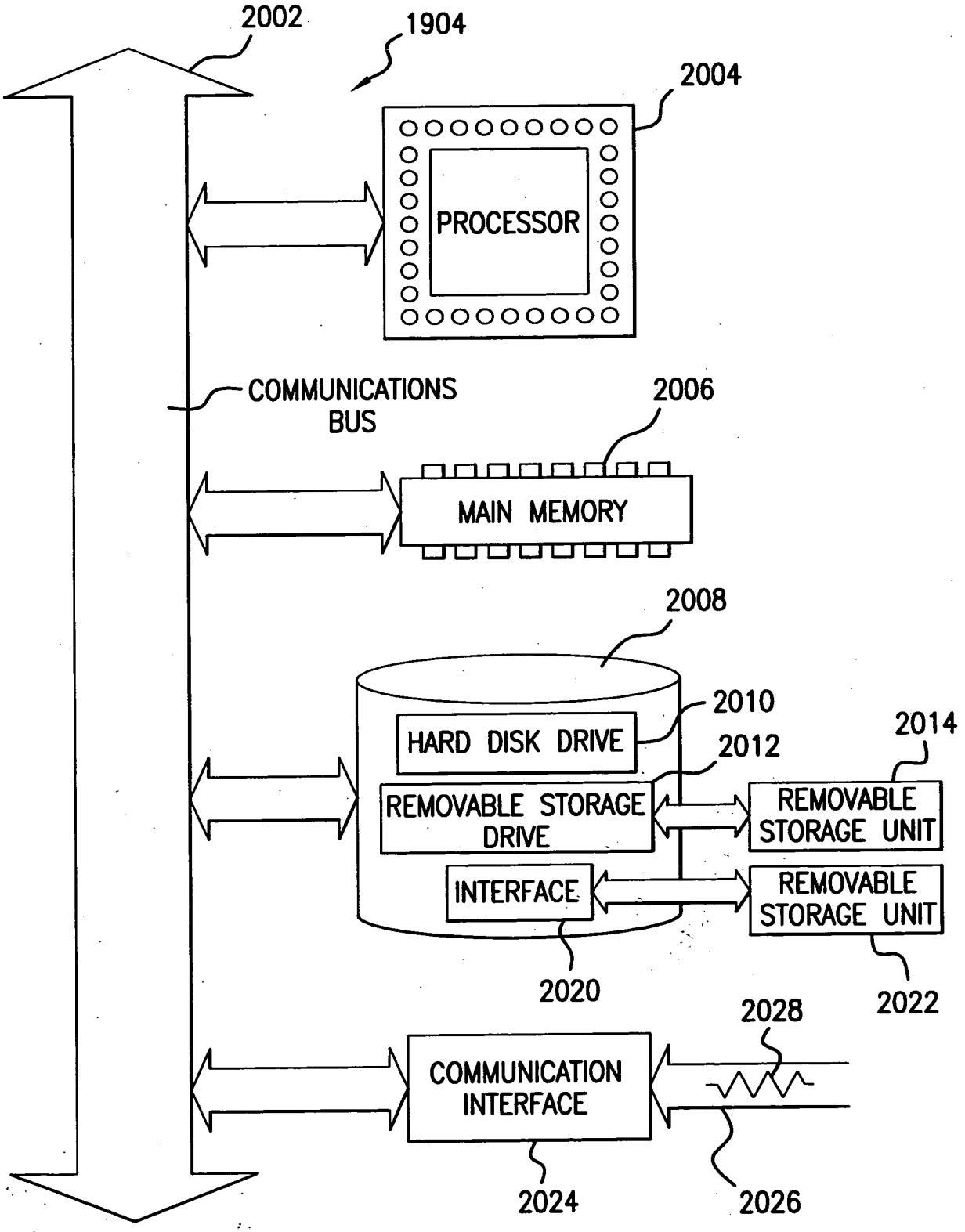

FIG.20

APPROVED | O.G. FIG.
BY | CLASS | SUBCLASS
DRAFTSMAN

Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov *et al.*; Tel: 202/371-2600
Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries

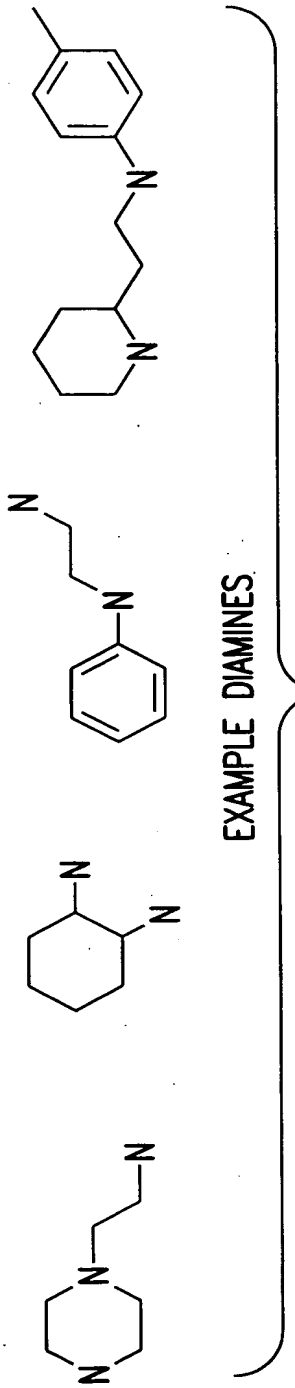

FIG.21A

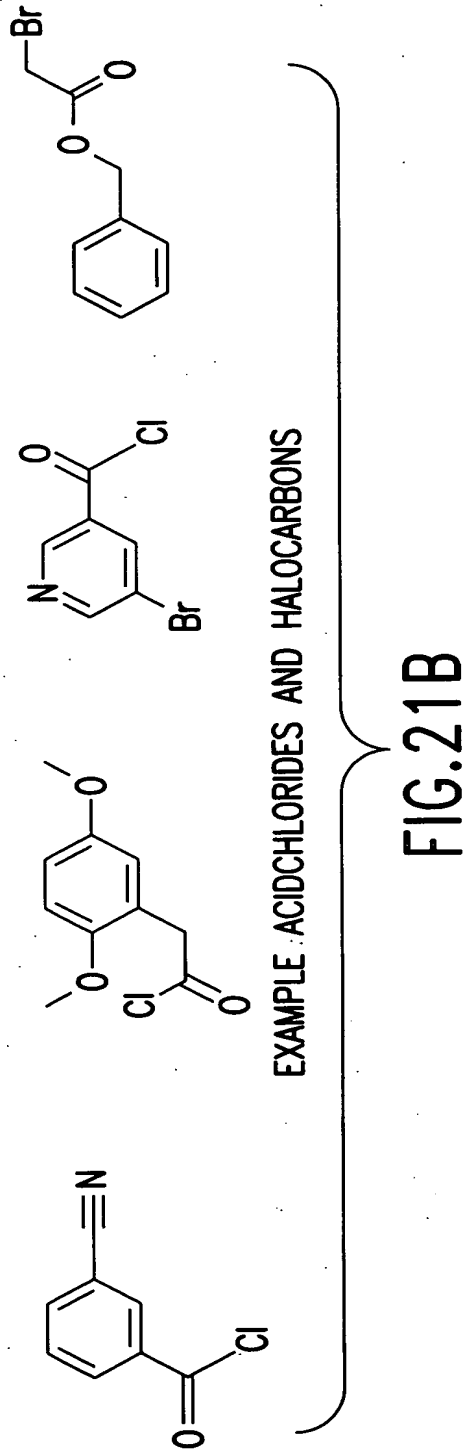

FIG.21B

APPROVED O.G. FIG.
BY CLASS SUBCLASS
DRAFTSMAN

Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov *et al.*; Tel: 202/371-2600
Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries

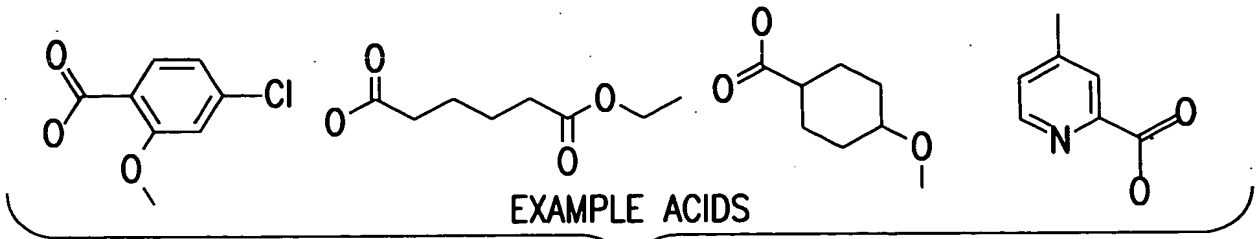

FIG.22A

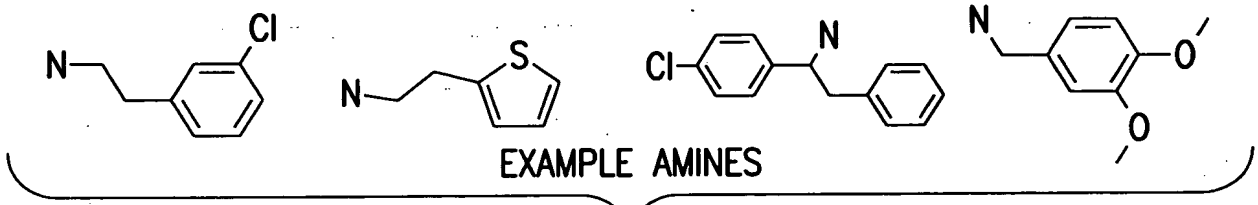

FIG.22B

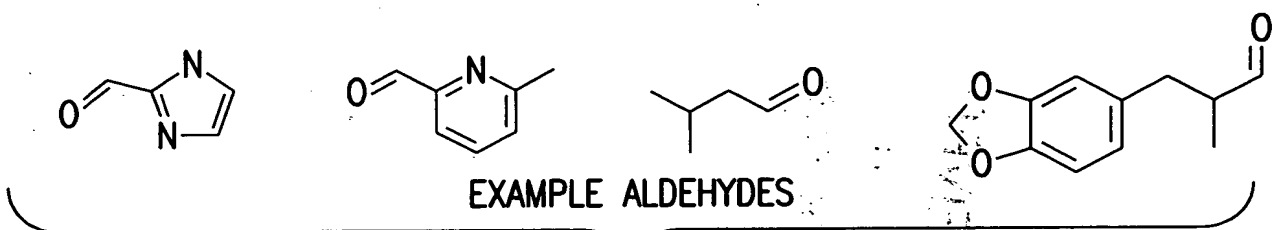

FIG.22C

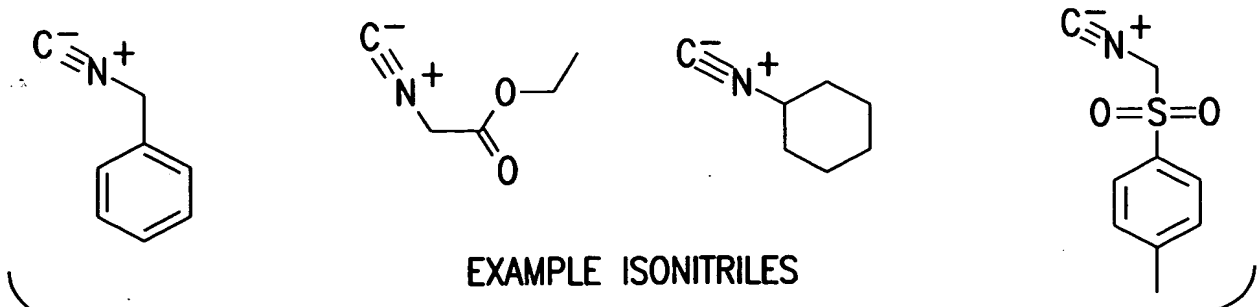

FIG.22D